## **Supplementary Material**

## Perspective

TNF Receptor Type II as an Emerging Drug Target for the Treatment of Cancer, Autoimmune Diseases, and Graft-Versus-Host Disease: Current Perspectives and *In Silico* Search for Small Molecule Binders

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Supplementary Figure 1 (a) | TNFR2 region 3 binders. ZINC72321887:(1R,2S,3R,4R)-3-[(6-methoxy-3-pyridyl)methylamino]-4-pyrimidin-5-yl-cyclopentane-1,2-diol, ZINC67911837: 4-amino-2-hydroxy-5-[[1-hydroxy-1-(5-oxo-6-bicyclo[4.1.0]hept-3-enyl)propan-2-yl]amino]-5-oxopentanoic acid, ZINC01611597: N-[3-(1-methyl-5-oxo-2-sulfanylideneimidazolidin-4-yl)propyl]guanidine, ZINC77265363:N-[[(2R,3S,4R)-3-hydroxy-4-(oxetan-3-ylamino)tetrahydrofuran-2-yl]methyl]thiophene-2-carboxamide, ZINC20465842: [(2R,3R,4S,5S)-4-hydroxy-5-(hydroxymethyl)-3-[methyl(2-pyridin-2-ylethyl)amino]oxolan-2-yl]methylazanium, RRA: Arginine, Arginine and Alanine

**Supplementary Figure 1 (b)** | TNFR2 region 4 binders. ZINC71316232: methyl (3R,4R,5R)-3-[(Z)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxy-1,4,5-trihydroxycyclohexane-1-carboxylate, ZINC01532677:(2R,4S,5S,6R)-6-methyloxane-2,3,4,5-tetrol, ZINC00281472: (2S,3S)-3-(1H-benzimidazol-2-yl)-2,3-dihydroxypropanoic acid